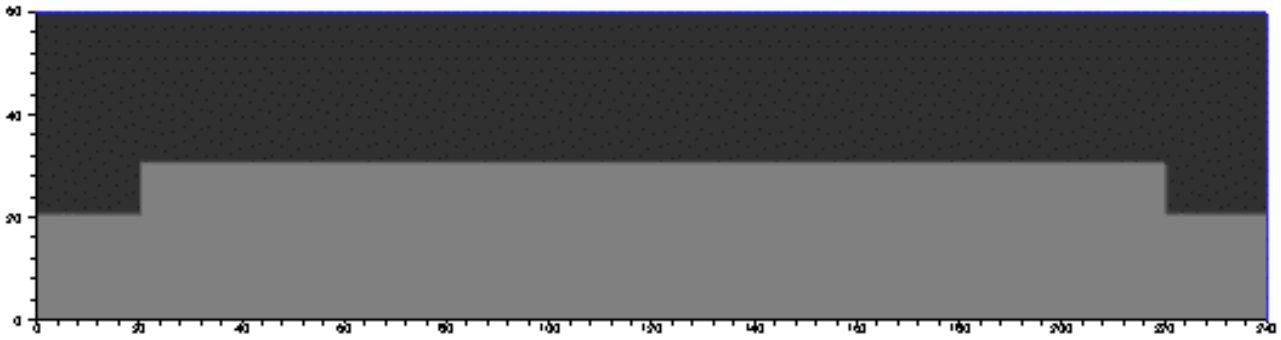
Diffusional Phase Transformations in Small Systems

W.C. Johnson and J.M. Howe, University of Virginia, DMR Award#9902110

Self-organization of Nanoparticle Arrays

- Patterned substrate and surface bias phase decomposition
- Compositional and epitaxial strains alter particle positions, size, and spacing
- Film composition controls microstructure and number of particles
- Elastic effects influence stability of microstructure
- Important for electronic device applications and growth and alignment of quantum dot structures



Simulation

Black: A-rich phase
White: B-rich phase
Gray: substrate

Simulation information: Gray area is the patterned substrate and the initially black area is the alloy film. The film composition lies just outside the spinodal composition. Decomposition proceeds by segregation to the substrate and then spinodal decomposition in this enriched area. The film is under compression in this example. The white areas are rich in component B and the dark areas rich in component A. (Regular solution model.) This same model can be applied to III-V compounds.

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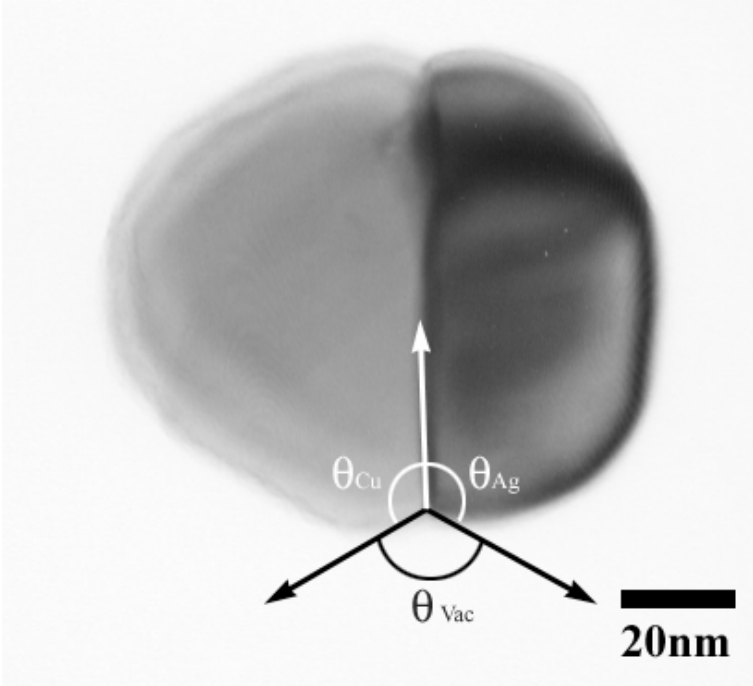
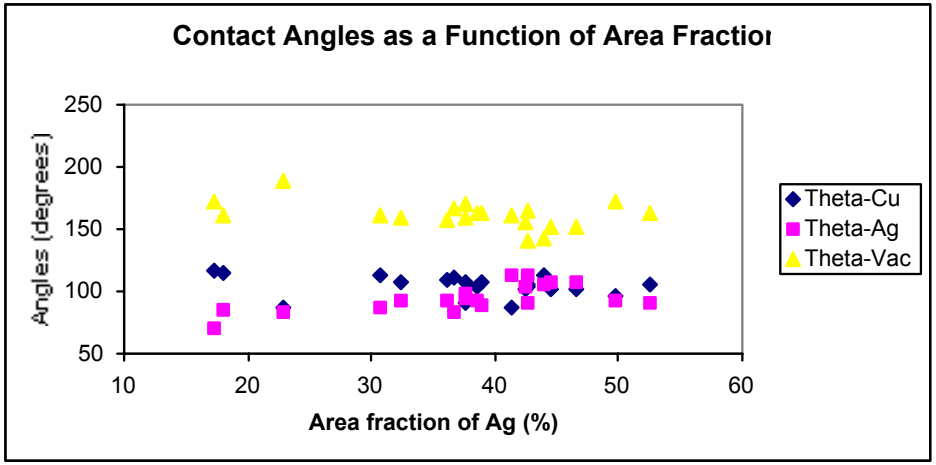
Training and Outreach:

- Graduate students:
  - S.M. Wise (theory)
  - K. Chatterjee (experiment)
- Fulbright Fellow: Dr. A. M. Mebed (Egypt)
- Co-organizer of 2002 Gordon Conference (JMH)
- ASM Research Silver Medal 2000 (JMH)
- Organized materials theory group of undergraduate engineers (WCJ)
- All-University Outstanding Teaching Award 1999 (WCJ)
- Fellow of ASM 2000 (WCJ)

Small Particles

- Contact angles at three-phase junction vary with volume (area) fraction of phases in two-phase particles
- Ag-Cu two-phase particles have semicoherent {111} interphase boundaries, similar to those in bulk alloys





The contact angles at a three-phase junction are determined by a balance among the surface and interfacial energies and assume a constant value at equilibrium in bulk alloys. In contrast to this, the contact angles vary with the volume fraction (projected area fraction in TEM) of the phases in small two-phase particles. As shown in the graph for two-phase Ag-Cu particles, the contact angle of the Ag phase (dark in TEM image) increases with its volume fraction, with corresponding decreases in contact angles of the Cu and vapor phases. Initial modeling results of this phenomena give good agreement with the experimental observations.

Dr. Mebed's research has been supported by this grant. He is a Fulbright Fellow from Egypt working with WCJ and JMH on phase decomposition in Cu-Co thin films and is also involved with the experimental work depicted on this page.